

ADVANCED MODELING TECHNIQUES FOR IMPROVED SNCR CHEMISTRY APPLICATION FOR NO_x CONTROL IN UTILITY BOILERS

M. A. Cremer, D. A. Swensen, M. K. Denison, M. J. Bockelie, and M. P. Heap
Reaction Engineering International
Salt Lake City, UT

At present, detailed SNCR computer simulations for utility boilers are complex and intensive. It is difficult to accurately model the detailed chemistry associated with SNCR systems and take account of turbulence interactions. The detailed mechanism REI uses contains over 60 chemical species and 250 reversible steps, and implementation of this detailed chemical mechanism into our CFD codes requires the solution of transport equations for the same number of species as exist in the mechanism. This is prohibitive from the standpoint of both CPU time and memory. Thus, a reduced description of the detailed chemistry is necessary. In addition, it is difficult to control the direction of the simulation at run time, to visualize the solution as it is evolving and to determine optimum input configurations such as reagent injector locations.

In response to these problems, REI is pursuing two significant advances in computational procedures. The first is the application of a Computer Assisted Reduction Method (CARM) which automates the chemical mechanism reduction process and calculates the chemical source terms defined by the reduced mechanism. The second is an SNCR analysis tool that provides the ability to visualize and interrogate the reacting flow solution as it evolves, and then immediately make modifications to model parameters. In addition, a neural network and a constrained optimization algorithm have been integrated to help guide the user to optimum input configurations. This paper will present results of recent boiler modeling studies using CARM and computational steering.